Enhanced sensitivity to the fine-structure constant variation in Th IV atomic clock transition

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Our calculations have shown that the $5f_{5/2} - 7s_{1/2}$ 23131 cm^{-1} transition from the ground state in the ion Th^{3+} is very sensitive to the temporal variation of the fine structure constant $\alpha = e^2/\hbar c$ ($q = -75300$ cm^{-1}). The line is very narrow, the ion has been trapped and laser cooled and the positive shifter line $5f_{5/2} - 5f_{7/2}$ 4325 cm^{-1} ($q = +2900$ cm^{-1}) may be used as a reference. A comparison may also be made with a positive shifter in another atom or ion. This makes Th^{3+} a good candidate to search for the α variation.

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I. INTRODUCTION

Theories unifying gravity with other interactions suggest temporal and spatial variation of the fundamental "constants" in expanding Universe (see e.g. review [1]). The spatial variation can explain fine tuning of the fundamental constants which allows humans (and any life) to appear. We appeared in the area of the Universe where the values of the fundamental constants are consistent with our existence. The fundamental constants may be slightly different near massive bodies (see e.g. review [2]). There are some hints for the variation of different fundamental constants in quasar absorption spectra [3, 4, 5, 6, 7, 8] and Big Bang nucleosynthesis [9, 10] data. However, a majority of publications report limits on the variations of the fundamental constants (see e.g. reviews [11, 12]).

The dependence of atomic transition frequencies on α may be presented in the following form

$$\omega = \omega_{\rm lab} + qx, \quad x \equiv (\alpha/\alpha_{\rm lab})^2 - 1\,. \tag{1}$$

In [13, 14], it was proposed to use transitions with significantly different q factors for astrophysical and laboratory measurements of α variation. One can search for a variation of α by comparing two frequencies of atomic transitions over a long period of time. Following the Ref. [15] we can represent a measured quantity $\Delta(t)$ as

$$\Delta(t) = \frac{d\ln(\omega_1/\omega_2)}{dt} = \left(\frac{\dot\omega_1}{\omega_1} - \frac{\dot\omega_2}{\omega_2}\right), \tag{2}$$

where $\dot\omega \equiv d\omega/dt$. Taking into account Eq. (1) we can rewrite Eq. (2) as follows

$$\Delta(t) \approx \left(\frac{2q_1}{\omega_1} - \frac{2q_2}{\omega_2}\right)\left(\frac{\dot\alpha}{\alpha_{\rm lab}}\right). \tag{3}$$

Narrow transitions with large and different q values are of experimental interest.

Note that the atomic unit of energy cancels out in the ratio of two transition frequencies. The α dependence appears due to the relativistic corrections which rapidly increase with the nuclear charge Z, $\sim Z^2\alpha^2$, and strongly depend on the electron angular momentum. Therefore, transitions in heavy atoms with larger electron angular momentum difference (like $\Delta l = 2$ for s and d orbitals) have larger q-coefficients. At present the best laboratory constraint on the temporal variation of α of $\dot\alpha/\alpha = (-1.6 \pm 2.3) \times 10^{-17}$ yr^{-1} was obtained by Rosenband *et al.* in Ref. [16] by comparing the frequencies of the the $^2S_{1/2} \to {}^2D_{5/2}$ transition in $^{199}Hg^+$ ($q = -52200$ cm^{-1}) and $^1S_0 \to {}^3P^o_0$ transition in $^{27}Al^+$ ($q = 146$ cm^{-1}).

The relativistic corrections also rapidly increase with the effective charge $Z_{\rm eff}$ which an external electron "sees". These corrections are proportional to $Z^2_{\rm eff}$. In the case of one electron above closed shells $Z_{\rm eff} = Z_i + 1$ where Z_i is the ion charge. Therefore, highly charged ions are expected to have larger q. Unfortunately, the interval between the energy levels also increases $\sim Z^2_{\rm eff}$, therefore, there is a risk to be out of the laser range. However, the Coulomb degeneracy and configuration crossing phenomena may help here. Indeed, in a neutral atom an electron energy level with larger orbital angular momentum is significantly higher than a level with lower orbital angular momentum with the same principal quantum number n.

For example, in the neutral Th the $5s$ electron is a core electron while the $5f$ electron is a valence electron. Respectively, the one-electron energy of the $5f$ electron is much higher than that of the $5s$ electron. Moreover, it is even higher than the energy of the $7s$ electron. As seen from the experimental spectrum of the energy levels of the neutral (four-valence) Th [17], the energy of the $6d^27s5f$ state is higher than the energy of the $6d^27s^2$

state. In the hydrogen-like Th the energy of the $5f$ state is equal to the energy of the $5s$ state, i.e. it is significantly lower than the energy of the $7s$ state. Therefore, there should be an ion charge at which the level $5f$ "crosses" the level $7s$ (at some higher charge it crosses $6s$, etc). This kind of an approximate crossing (between the $5f6d$ and the $6d7s$ states) happens in Th^{2+}, where the interval between them is about 5500 cm^{-1} only. The interval between the $5f$ and $7s$ states in Th^{3+} is also relatively small. Finally, the lifetime of the excited state should be large to have a narrow line.

All these requirements clearly point towards the $5f_{5/2} - 7s_{1/2}$ (23131 cm^{-1}) transition in Th^{3+}. It is also very important that the laser cooling of the $^{232}Th^{3+}$ ion has recently been reported by Campbell *et al.* in their paper [18]. This was the first time when a multiply charged ion has been laser cooled.

According to our calculations presented below the $5f_{5/2} - 7s_{1/2}$ transition is a negative shifter with $q = -75300$ cm^{-1}. Another narrow line in the same ion is the positive shifter $5f_{5/2}-5f_{7/2}$ (4325 cm^{-1}) with $q = +2900$ cm^{-1}, this line may be used as a reference. Comparison may also be made with a positive shifter in another element, where q may exceed 30000 cm^{-1} (see the table of atomic clock transitions with q coefficients in review [19] and recent work [20]).

II. METHOD OF CALCULATION

To find q factors we need to solve the atomic relativistic eigenvalue problem for different values of α or, respectively, for different values of x from Eq. (1). The value of x was chosen to be equal to $|x| = 1/8$. This is a convenient choice that allows us to neglect nonlinear corrections and, on the other hand, to make calculations numerically stable. Thus, we need to calculate atomic frequencies $\omega_\pm$ for two values $x = \pm 1/8$. The corresponding q factor is given by

$$q = 4(\omega_+ - \omega_-). \tag{4}$$

Since Th^{3+} is a univalent ion we have carried out calculations of its energy levels in the frame of the Dirac-Hartree-Fock (DHF) method combined with many-body perturbation theory (MBPT). The latter allows us to take into account correlations between the valence electron and the core electrons.

We start from solving the DHF equations in the V^{N-1} approximation. On the first stage the electrons of the closed core were included in a self-consistency procedure and their orbitals were found. After that we constructed the valence orbitals for several low-lying states using the frozen-core DHF equations. The virtual orbitals were determined with the help of a recurrent procedure described in [21]. The one-electron basis set of the following size was constructed: $1-20s$, $2-20p$, $3-20d$, $4-25f$, $5-18g$.

TABLE I: The low-lying energy levels (in cm^{-1}) in the DHF and the DHF+Σ approximations are presented. The theoretical values are compared with the experimental data.

DHF		DHF+Σ		Experiment[a]
$6d_{3/2}$	—	$5f_{5/2}$[b]	—	—
$6d_{5/2}$	4225	$5f_{7/2}$	4800	4325
$5f_{5/2}$	5190	$6d_{3/2}$	9003	9193
$5f_{7/2}$	8617	$6d_{5/2}$	14749	14486
$7s_{1/2}$	11519	$7s_{1/2}$	21371	23131
$7p_{1/2}$	46702	$7p_{1/2}$	59487	60239
$7p_{3/2}$	58225	$7p_{3/2}$	72690	73056
$8s_{1/2}$	102595	$8s_{1/2}$	120106	119622
$7d_{3/2}$	103148	$7d_{3/2}$	120844	119685
$7d_{5/2}$	104763	$7d_{5/2}$	122603	121427
$6f_{5/2}$	111874	$6f_{5/2}$	128763	127262
$6f_{7/2}$	112316	$6f_{7/2}$	129251	127815
$8p_{1/2}$	117185	$8p_{1/2}$	135165	134517
$8p_{3/2}$	122194	$8p_{3/2}$	140552	139871
$9s_{1/2}$	142328	$9s_{1/2}$	161485	160728

[a]Reference [17];
[b]The removal energy of the $5f_{5/2}$ state was found to be equal to 0.9414 au on the DHF stage and 1.0578 au on the (DHF+Σ) stage. The experimental value is 1.0588 au.

At the next stage we included core-valence correlations (Σ) into consideration and the wave functions were determined by solving the equation

$$H_{\rm eff}(E_n)\,|\Psi_n\rangle = E_n\,|\Psi_n\rangle\,, \tag{5}$$

with an effective Hamiltonian defined as

$$H_{\rm eff}(E) = H_{\rm FC} + \Sigma(E)\,, \tag{6}$$

where $H_{\rm FC}$ is the frozen-core DHF Hamiltonian and the self-energy operator Σ is the energy-dependent correction, involving core excitations. In the following we will refer to it as the DHF+Σ formalism.

III. DISCUSSION AND RESULTS

In Table I we list the low-lying energy levels and compare them with the experimental data. To stress an importance of accounting for the core-valence correlations we present in Table I the results obtained on the stage of pure DHF approximation and in the frame of DHF+Σ formalism.

As seen from Table I on the DHF stage even the order of the low-lying levels is incorrect. For instance, the $6d_{3/2}$ state lays deeper than the $5f_{5/2}$ state. An agreement between theoretical and experimental energy levels is rather poor. An accounting for the core-valence correlations (Σ corrections) recovers the correct order of the states. Besides that the theoretical energy levels become much closer to the experimental values.

To find the q factors of the excited states in respect to the ground state $5f_{5/2}$ we need to carry out calculations of frequencies $\omega_\pm$ for two values $x = \pm 1/8$. These

TABLE II: The values of the q factors (in cm^{-1}) found in the DHF+Σ approximations are presented.

	q
$5f_{5/2}$	—
$5f_{7/2}$	2900
$6d_{3/2}$	-39000
$6d_{5/2}$	-34300
$7s_{1/2}$	-75300
$7p_{1/2}$	-67000
$7p_{3/2}$	-48900
$8s_{1/2}$	-57500
$7d_{3/2}$	-50600
$7d_{5/2}$	-46900
$6f_{5/2}$	-46100
$6f_{7/2}$	-45500
$8p_{1/2}$	-57300
$8p_{3/2}$	-50000
$9s_{1/2}$	-55100

calculations are similar to those carried out for the laboratory value of the fine structure constant $\alpha_{\rm lab}$. For this reason we do not discuss them in detail. We only stress again that it is important to include the Σ corrections for obtaining the correct values of the frequencies $\omega_\pm$ and, respectively, the correct values of the q factors.

In Table II we present the q factors of the excited states listed in Table I in respect to the ground state, obtained on the DHF+Σ stage. As follows from Eq. (4) the accuracy of the q factors corresponds to the accuracy of calculations of ω_+ and ω_-. The spectrum of the energy levels of Th^{3+} is not too dense and we believe that the energy levels obtained at α_+ and α_- are found with the same accuracy as the energy levels computed at $\alpha_{\rm lab}$. As seen from Table I the latter are reproduced within the 10% accuracy. Correspondingly, the accuracy of the q factors can also be estimated at the level of 10%.

As seen from Table II almost all q factors are negative. As expected, the largest q factor in absolute value was found for the $5f_{5/2} - 7s_{1/2}$ transition. The only positive q factor was obtained for the $5f_{5/2} - 5f_{7/2}$ transition.

The transition frequency between fine structure levels of one multiplet $\omega_{J,J-1}$ (where J is the total angular momentum) in the first order in $(\alpha Z)^2$ is given by the well known Landé rule: $\omega_{J,J-1} = AJ(\alpha Z)^2$. It directly leads to $q_{J,J-1} = \omega_{J,J-1}$ (see Eq. (1)).

A marked difference between $q(5f_{5/2} - 5f_{7/2}) = 2900$ cm^{-1} and $\omega(5f_{5/2} - 5f_{7/2}) = 4325$ cm^{-1} demonstrates an importance of the second order relativistic corrections $\sim (\alpha Z)^4$ for Th. These corrections modify the expression for $\omega_{J,J-1}$ leading to (see, e.g., [22])

$$\omega_{J,J-1} = AJ(\alpha Z)^2 + (B_J - B_{J-1})\,(\alpha Z)^4\,, \qquad (7)$$

where A and B_j are certain coefficients and B_j are not small in comparison with A.

Since Th is the heavy element with $Z = 90$, the parameter (αZ) is not small for it. In particular, $(\alpha Z)^4 \approx 0.2$ and the term $\sim (\alpha Z)^4$ gives a noticeable contribution to the $q(5f_{5/2} - 5f_{7/2})$.

To conclude, we have calculated the q factors for a number of excited states in Th^{3+} in respect to the ground state $5f_{5/2}$. Our calculations showed that the $q(5f_{5/2} - 7s_{1/2})$ is very large in absolute value and, respectively, the $5f_{5/2} - 7s_{1/2}$ transition is very sensitive to the temporal variation of the fine structure constant. Since the $7s$ state is a metastable state, this transition is convenient for an experimental laboratory search of α variation. Another transition $(5f_{5/2} - 5f_{7/2})$ can be used as a reference.

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